Accelerated Strategic Computing Initiative

ASCI at Livermore

University of California • Lawrence Livermore National Laboratory

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Tri-Lab ASCI Preparations Begin for SC2001 Conference Exhibit

Preparations are underway for Tri-Lab ASCI participation in *SC2001*—the annual supercomputing conference to be held November 10–16, 2001 in Denver, Colorado.

ASCI scientists are urged to visit the "ASCI Exhibit at SC2001" website and consider exhibiting or demonstrating their projects. Our Tri-Lab website at http://www.sandia.gov/supercomp/index.html will tell you more about project requirements and deadlines. In addition, you can reserve a space and fill out a participant application form even if your plans are incomplete at this point.

The *SC2001* submission deadline is August 31, 2001. If you have questions, please get in touch with LLNL's point of contact: Jean Shuler at Extension 3-1909 or jshuler@llnl.gov.

The ASCI Program uses this annual *SC2001* conference series to feature many of its most impressive challenges and accomplishments, and to showcase significant contributions to high-end technical computing. The ASCI research exhibit is an imposing and popular booth that enjoys high visibility and excellent traffic. Scientists, engineers, students, designers, managers,

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ASCI's Power Wall in Building 451 Supports Unclassified Research

This is the third in a series of articles about ASCI Power Walls at LLNL. In Issue 2 of ASCI at Livermore*, Terri Quinn discussed the features and value of the Data Assessment Theater in B132N. In Issue 3, Steve Langer described the Visualization Work Center recently dedicated in B111.*

In October 2000, ASCI activated a new power wall in the B451 White Room, which allows for unclassified visualization presentations on a 6-video-cube, 2 × 3 array. Each cube is a self-contained projection unit and screen, similar to a home projection television, except that each screen has approximately 4.3 times the resolution of a home TV. The purpose of this power wall is to provide a means of presenting and studying the results of large unclassified scientific visualizations from computed data to groups of scientists and collaborators.

The display is driven by a 24 gigaflop (GF), 48-processor Silicon Graphics (SGI) computer with 5.5 terabytes (TB) of disk storage. The single screen resolution achieves 1280 pixels horizontal by 1024 pixels vertical. The total display resolution is 3840 pixels horizontal by 2048 pixels vertical, for a total display pixel count of 7,864,320 pixels. For comparison, a typical TV displays about 307,000 visible pixels.

The B451 White Room video cube display is a smaller, unclassified

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Phil Duffy (center), from the Atmospheric Science Division, illustrates some of his Multi-Programmatic and Institutional Computing climate modeling research for Tech TV reporter Bob Hirschfeld and cameraman Chris Kievman. Duffy's work was part of a variety of simulations from several programmatic areas, which were presented on ASCI's B451 Power Wall.

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Power Wall...*Continued from page 1*

version of the 15-projector classified system (using Electrohome LCD projectors) assembled just over two years ago in B132N. That system displays approximately 19.7 million pixels on a 16- × 8-ft screen. It is driven by a 32-GF SGI computer with 9 TB of high performance disk storage.

The modular architecture of the B451 video cubes, which requires minimal periodic alignment, allows for rapid deployment of this first unclassified power wall facility at LLNL.

ASCI has inspired a great deal of large scale computing, some of which is not directly related to weapons work. Many of the presentations at LLNL's *Science Day* included research into climate modeling, earthquake prediction, astrophysics, and computational biology.

In May, this unclassified power wall was used for presentations during CASC's University of California Review and for recent news coverage about LLNL research. As shown on page 1, Phil Duffy from the Climate and Carbon Cycle Modeling Group in Atmospheric Sciences discussed current climate modeling research with reporters from Tech TV. In addition, David Nowak used the B451 Power Wall to explain the simulation of a high explosive detonation at the atomistic level to a TV audience (see the replay of the Tech TV broadcast on our website at http://www.llnl.gov/asci/news/issue4_01.html)

Tech TV's anchor Victoria Recano introduces David Nowak, who used the B451 Power Wall to visualize the carbon, nitrogen, oxygen, and hydrogen atoms and their bonds in a high-explosive simulation.

Mary Zosel Begins ASCI D.C. Assignment

SCCD's Mary Zosel has completed the first month of her assignment in Washington, D.C.

Mary Zosel has agreed to serve as technical advisor to the Director of the Office of Advanced Simulation and Computing (DP-14) under the Deputy Assistant Secretary for Research, Development and Simulation (DP-10) in Washington, D.C. Her assignment will be for one year starting May 1, 2001 with a possible extension for the following year.

Mary, a member of the Computation Directorate and assigned to Livermore Computing in the Scientific Computing and Communications Department, will remain in the Computation Directorate administratively and will report programmatically to the Defense and Nuclear Technologies Directorate.

She will provide technical input to NNSA/DP program managers in technical reviews, technical assessments of progress, strategic planning and implementation of the ASCI Program. She will act as technical interface and assist in coordinating the ASCI platform program planning activities and associated facility issues. Mary will serve as a participating member of the NNSA/DP-14 Advanced Simulation and Computing team.

Mary earned her Ph.D. in Computer Science at the University of Washington in 1971 and joined Livermore Computing the same year. Her research interests include parallel and distributed code development, tools, parallel computer architecture, and general high performance computing. She has been part of the ASCI PSE effort since the beginning of the ASCI Program.

Mary is currently the PI for ASCI Simulation Development Environment and the Deputy LLNL Lead for PSE. She serves as the LLNL representative on the ASCI Alliance Tri-Lab Sponsor Team for the University of Utah and has participated in the PathForward Ultrascale Tools Initiative and in platform procurement activities for several ASCI systems.

High-explosive Simulations in ASCI Reveal the Role of Defects

Ironically, plastic-bonded explosives are precision materials because of their defects or voids. When the void volume of HMX (tetranitro tetrazacyclo-octane) explosives is too small, the minimum pressure required to ignite them becomes too high to be practical. When the void volume is too large, the explosives are too sensitive. In the past, these defects were engineered using empirical rules and testing. Now we can examine the role of such defects computationally.

The cube shown in Fig. 1 measures 100 μm on a side and contains about 100 grains of HMX represented in various shadings, and includes a light-colored fluorocarbon polymer binder tradenamed Viton. In the simulation, we have inserted voids to make 1% porosity by volume at locations where three or more particles meet. The voids look like deflated soccer balls. This cube has the composition of LX-04, an explosive developed at LLNL—HMX 85%/ Viton 15% by weight with 1% to 2% porosity by volume.

We remove all of the binder and some of the particles to show voids located between the HMX grains (Fig. 2). Next, we remove all of the HMX particles, leaving only the voids visible (Fig. 3). A 120-kbar shock is applied to one face of the cube. This pressure is below the threshold for HMX reaction in the absence of voids for both the calculation and for experiments on HMX single crystals. Figure 4 shows the shock wave as it sweeps over the void from right to left. Far from the void, the HMX material is heated somewhat by the passage of the shock; near the void, plastic deformation forces the HMX into the space where the void once was, causing additional heating.

In the wake of the shock, the hot spots, shown in Fig. 4 are temperature contour surfaces that enclose material hotter than 900 K. These hot spots appear where voids used to be. The material in those regions is chemically reacting to form gas products. At this pressure, the density of the gas products is about 1.50 g/cm^3; the original LX-04 density is 1.85 g/cm^3.

This simulation was performed with ALE-3D, and used heat transfer and thermally driven chemical reactions in addition to elastic-plastic-hydrodynamic flow to describe the early stages of explosive ignition. The calculation used 3.5 million zones, was performed on the Tera Cluster with 128 processors, and took 500 hours of computing time.

See the QuickTime movie of this HE simulation on our *ASCI at Livermore* web page at http://www.llnl.gov/asci/news/issue4_01.html

—J. E. Reaugh and S. C. Keeton

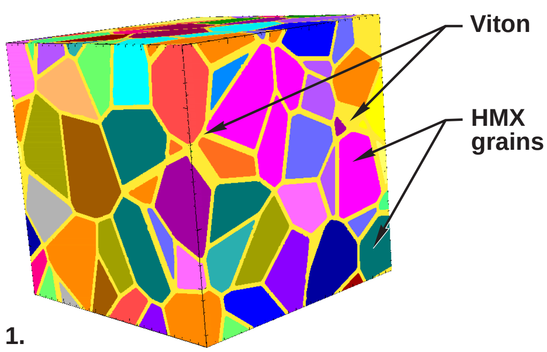

Figure 1. Grain-scale simulations. The cube is 100 μm on a side and contains shaded grains of HMX and a light-colored binder called Viton.

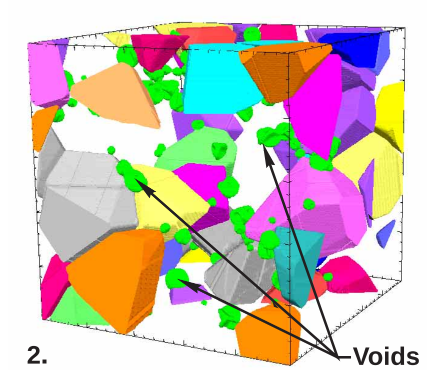

Figure 2. The cube with the binder and some HMX grains removed. The voids are located between some of the HMX grains.

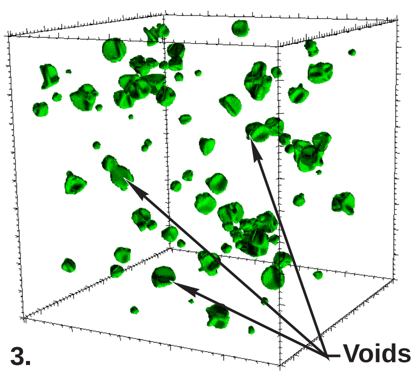

Figure 3. The cube with all the HMX and binder removed, showing all the voids.

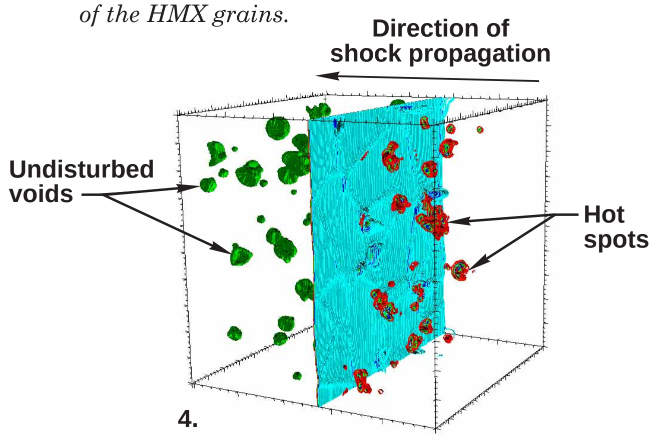

Figure 4. The shock wave moves through the cube, leaving hot spots where the voids used to be.

This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

SC2001 Preparations...

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and executives from all areas of high-performance computing and networking report that they visit the exhibit year after year to learn about ASCI's progress and innovations. In addition to Tri-Lab ASCI Program research, the booth benefits from collaborative activities with the Alliances, the nation's defense complex, and our industry partners.

"Beyond Boundaries," the *SC2001* theme, resonates particularly well for ASCI this year. Plans are to promote ASCI by presenting current research and development in such important subject areas as future working environments for computations professionals, wireless communications, and novel strategies for deploying break-through research. These presentations and demonstrations will exploit innovative technologies designed, developed, and implemented within ASCI. Collateral materials (posters, fliers, and signs) will support the science and technology effort with coherent design and graphics. Booth activities will be captured on a CD-ROM for post-conference distribution, which allows the program to leverage the presentations and demonstrations for maximum return on the year's R&D investments.

Jean Shuler (center) discusses plans for the ASCI booth at SC2001 with editor Alane Alchorn and designer Dan Moore. Jean leads the Tri-Lab team, which will exhibit and demonstrate many of ASCI's latest contributions to high-end computing at SC2001, to be held on November 10–16 in Denver.

Booth visitors can expect to find a mix of general ASCI information and individually selected highlights. The distribution of ASCI logo articles will be used to acquire visitor information. Business cards and data from *SC2001* badge swipes will be collected in exchange for these logo items. We will create a database of visitors' names, affiliations, and contact information; following the conference, we will send an ASCI CD to each visitor.

In addition to the staff of scientists in the booth, knowledgeable greeters will welcome visitors courteously and promptly, while specialty scientists and engineers demonstrate or discuss program specifics. ASCI personnel will wear ASCI logo shirts.

For further information, please visit the *SC2001* home page at http://www.sc2001.org/index.shtml.

Acknowledgment

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